JOURNAL OF MOLECULAR SPECTROSCOPY

JMOSA 3

UNIVERSITY OF HAWAII LIBRARY
LIBRARY USE ONLY

VOLUME 41, 1972

Editors

Harald H. Nielsen K. Narahari Rao

Editorial Advisory Board

Amat
rge Bak
J. Bernstein
yce L. Crawford, Jr.
vid M. Dennison
vid A. Dows
H. Günthard
S. Gutowsky
Herzberg

Jon T. Hougen
K. K. Innes
Richard C. Lord
P.-O. Löwdin
Ross A. McFarlane
A. Mangini
M. Migeotte
Ian Mills

Yonezo Morino
Robert S. Mulliken
John G. Phillips
J. Plíva
H. L. Welsh
E. Bright Wilson, Jr.
Manfred Winnewisser
R. N. Zare

ACADEMIC PRESS

NEW YORK and LONDON

Copyright © 1972, by Academic Press, Inc.

ALL RIGHTS RESERVED

No part of this volume may be reproduced in any form by photostat, microfilm, by retrieval system, or any other means, without written permission from the publishers.

Made in the United States of America

JOURNAL OF MOLECULAR SPECTROSCOPY **41**, iii–v (1972)

CONTENTS OF VOLUME 41

NUMBER 1, JANUARY 1972

ANNA MAE WALSH BAKKE. A Molecular Structure Study of Dimethylmercury, Dimethylcadmium, Dimethylzinc and the Deuterated Compounds 1

G. B. FISH, G. J. CARTWRIGHT, A. D. WALSH, AND P. A. WARSOP. Rotational Structure in the $^1\Sigma_u^- \leftarrow {}^1\Sigma_g^+$ Transition of Cyanogen at 2200 Å 20

W. J. MITCHELL AND M. K. DEARMOND. High Resolution Spectra of Cr(III)–Sulfur Chelates 33

TAKAYOSHI KOBAYASHI, SABURO NAGAKURA, SATOSHI IWASHIMA, AND HIROO INOKUCHI. The Spectral Dependence of Fluorescence Decay Times Observed for the Benzo[g,h,i]perylene Crystal and Its Mixed Crystal with Perylene 44

HIROSHI MORITA AND SABURO NAGAKURA. Near-Infrared Spectra of Hydrogen-Bonded Cyclic Dimers of Some Carboxylic Acids 54

K. WIELAND, JOEL B. TELLINGHUISEN, AND A. NOBS. The Band Systems $E \rightarrow B$ (4000–4360 Å) and $F \rightarrow X$ (2530–2740 Å) of $^{127}I_2$ and $^{129}I_2$, and the Corresponding System E ↔ B of Br_2 and Cl_2 69

P. L. LEE AND R. H. SCHWENDEMAN. The Microwave Spectrum, Barrier to Internal Rotation, and Dipole Moment of Cyclopropyl Methyl Ketone 84

R. J. CORICE, JR., K. FOX, AND W. H. FLETCHER. Studies of Absorption Spectra of GeH_4 in the 2–17 μ Region 95

CH. V. S. RAMACHANDRA RAO. Redundant Forces and Compliance Constants 105

ROBERT L. COOK, FRANK C. DE LUCIA, AND PAUL HELMINGER. Millimeter and Submillimeter Wave Rotational Spectrum and Centrifugal Distortion Effects of D_2S 123

R. W. PETERSON AND T. H. EDWARDS. Analysis of ν_4 of CD_3Br 137

MANFRED WINNEWISSER AND BRENDA P. WINNEWISSER. Millimeter Wave Rotational Spectrum of HCNO in Vibrationally Excited States 143

ARTHUR G. MAKI. A High Resolution Study of *l*-type Resonance in Cyclopropane 177

J. BOTINEAU. Infrared Absorption of Methane at High Resolution Between 1225 and 1400 cm^{-1} 182

B. R. PARKER AND G. P. KHARE. Infrared Spectra of DNA: Correlation of Theoretical and Observed Frequencies 195

H. FAST AND H. L. WELSH. High-Resolution Raman Spectra of Acetylene, Acetylene-d_1, and Acetylene-d_2 203

Notes

Agostino Baldacci, Sergio Ghersetti, and K. Narahari Rao. Assignments of the $^{12}C_2H_2$ Bands at 2.1–2.2 μ 222

Harold Jones and R. F. Curl, Jr. Microwave Spectrum and Dipole Moment of Vinyltrifluorosilane 226

James K. G. Watson. The Numbers of Structural Parameters and Potential Constants of Molecules 229

Errata 231

Number 2, February 1972

Kamil Sarka. Anomalous Values of the Rotational Constants of the Parallel Bands Perturbed by Coriolis Resonance 233

Yves Grenie and Chantal Garrigou-Lagrange. Infrared Spectra of Glycine Isotopic Species Isolated in an Argon or Nitrogen Matrix 240

G. L. LeBel and J. D. Laposa. Luminescence of Benzonitrile, Monodeuterobenzonitriles, and Perdeuterobenzonitrile at 77°K in Polycrystalline Matrices 249

G. Varghese, S. N. Ghosh, and S. Paddi Reddy. Frequency Shifts of Quadrupolar Components of the Collision-Induced Fundamental Band of H_2 291

Robin M. Hochstrasser and Ta-Yuen Li. Spectral Manifestations of Nonradiative Processes in Azulene 297

Hiroaki Baba and Michio Kitamura. Molecular Association and Emission Spectra of Benzoic Acid 302

P. R. Bunker and J. M. R. Stone. The Bending-Rotation Hamiltonian for the Triatomic Molecule and Application to HCN and H_2O 310

William H. Kirchhoff. On the Calculation and Interpretation of Centrifugal Distortion Constants: A Statistical Basis for Model Testing: The Calculation of the Force Field 333

W. Good, R. J. Conan, Jr., A. Bauder, and Hs. H. Günthard. Microwave Spectra of Deuterium Substituted 2-Chloropropenes and the Conformation of the Methyl Group 381

M. Ogawa and S. Ogawa. Absorption Spectrum of CO in the Hopfield Helium Continuum Region, 600–1020 Å 393

Notes

J. T. Bell. New Absorption Bands for the Uranyl Ion 409

R. Jankow and J. N. Willis, Jr. Minimizing Emission Background in Laser Raman Spectroscopy 412

Ira W. Levin, Stanley Abramowitz, and A. Müller. Jahn–Teller Vibrations of ReF_6 415

Harutoshi Takeo, Eizi Hirota, and Yonezo Morino. Third-order Potential Constants and Dipole Moment of SeO_2 by Microwave Spectroscopy 420

Errata 423

Number 3, March 1972

G. Herzberg and Ch. Jungen. Rydberg Series and Ionization Potential of the H_2 Molecule 425

Rauno Anttila. Near-Infrared Spectrum of CD_3CN 487

Basil Curnutte and Jagdeesh Bandekar. The Intramolecular Vibrations of the Water Molecule in the Liquid State 500

Jon B. Bryan and Basil Curnutte. A Normal Coordinate Analysis Based on the Local Structure of Liquid Water 512

Gisbert Winnewisser. Millimeter-Wave Rotational Spectrum of HSSD. $^rQ_0$-Branch 534

J. A. Coxon. The Extreme Red Absorption Spectrum of Br_2, $A^3\Pi(1_u) \leftarrow X^1\Sigma_g^+$ 548

J. A. Coxon. Franck–Condon Factors and R-Centroids for Halogen Molecules–III. The $A^3\Pi(1) - X^1\Sigma^+$ System of $^{79}Br^{81}Br$ 566

V. S. Kushawaha, B. P. Asthana, and C. M. Pathak. Chemical Excitation of AsO 577

J. D. Simmons and J. K. McDonald. The Emission Spectrum of AlN 584

Notes

H. Hüber and G. A. Ozin. Matrix Raman Spectroscopy; The Lithium Atom–Oxygen Molecule Cocondensation Reaction 595

C. di Lauro. Matrix Elements of the Powers of Q and P Operators for the Isotropic Two-Dimensional Oscillator 598

Announcement 600

Author Index 601

Subject Index 602